

1/22

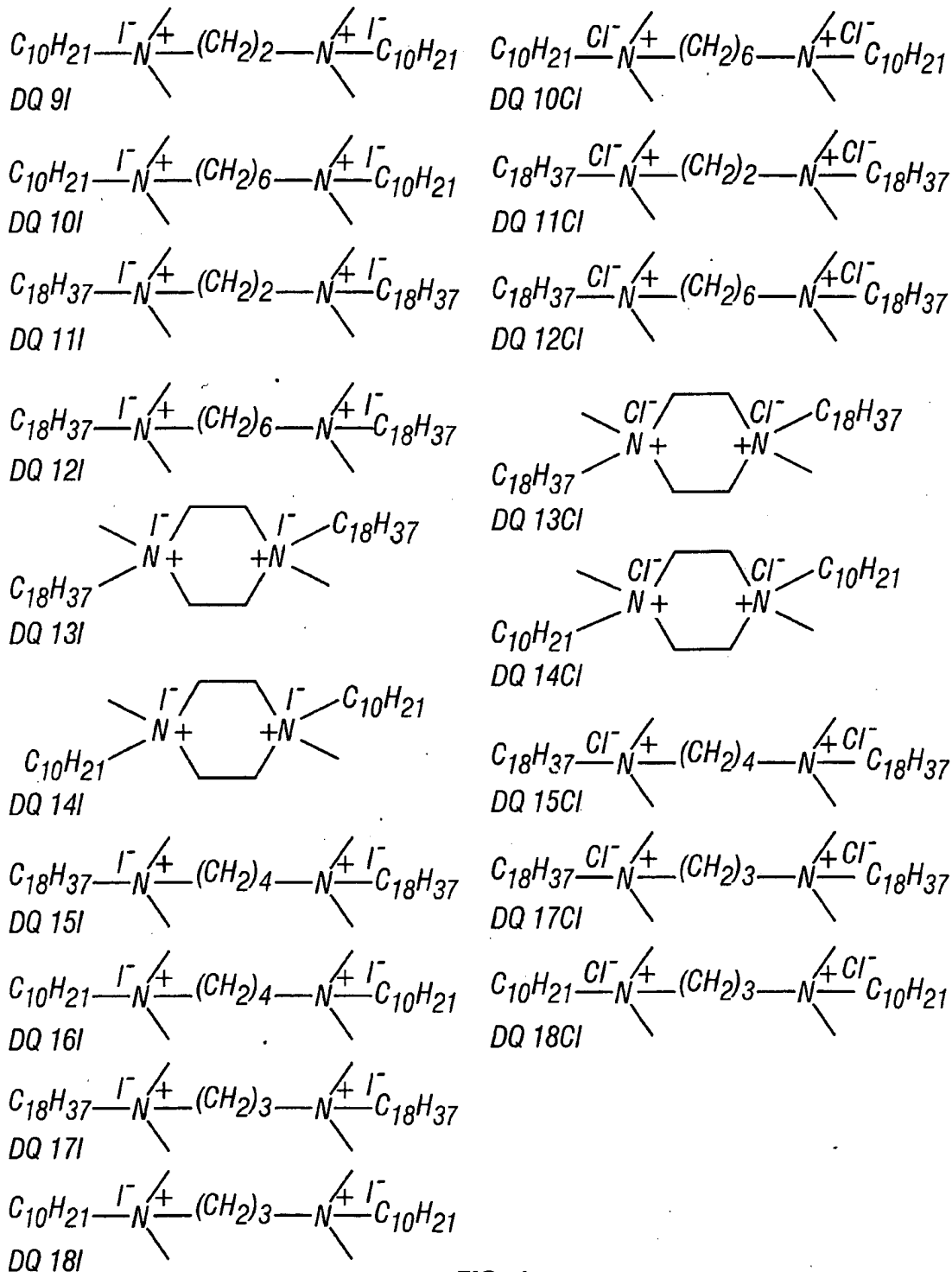


FIG. 1

2/22

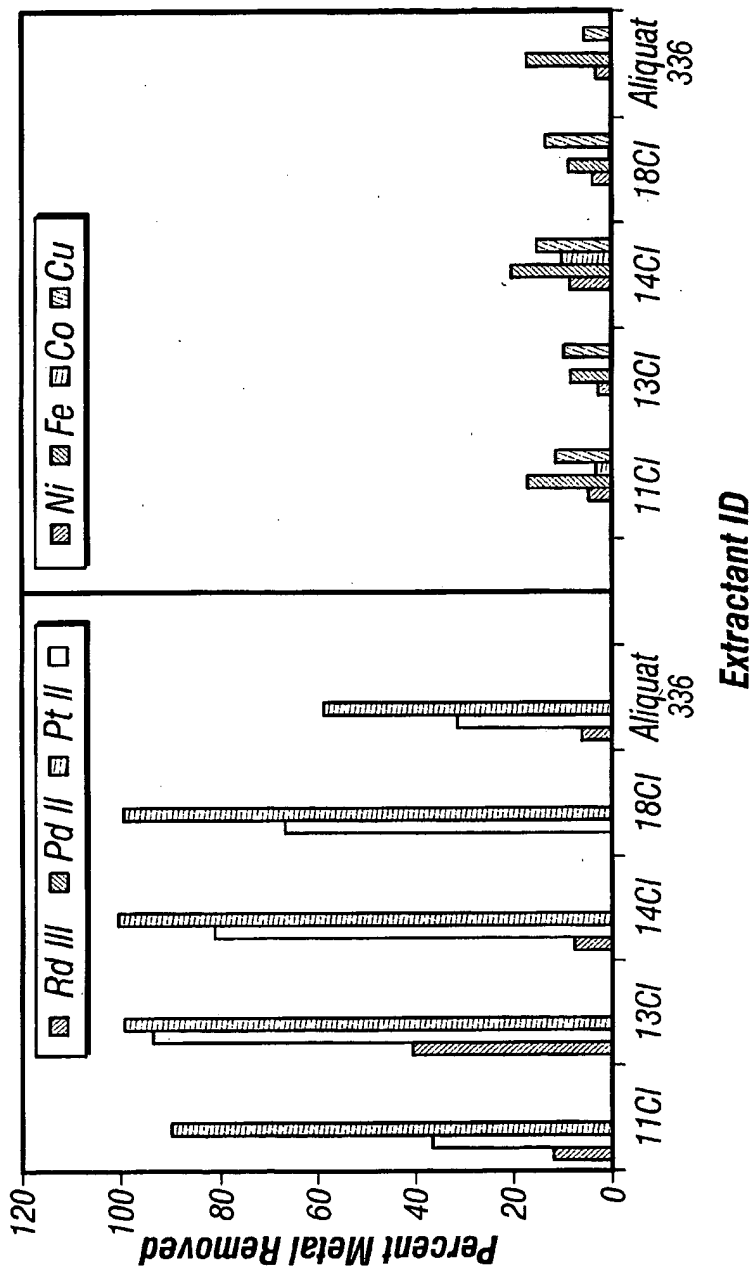


FIG. 2

3/22

Compound	D-Value Pd II	Conformation Minimum Energy (kcal/mole)	Connectivity Index (order 2, standard) D	Dipole Moment (debye) E	Electron Affinity (eV) F
DQ 18	2.86	39.331	11.632	12.744	7.127
DQ 16		39.449	11.985	2.933	6.601
DQ 10	1.75	40.322	12.692	0.01	5.948
DQ 14	2.6	39.924	11.071	25.323	8.122
DQ 17	3.3	50.797	17.289	25.52	7.139
DQ 15	0.42	49.902	17.642	0.025	6.597
DQ 12	1.59	50.899	18.349	0.124	5.946
DQ 13	3.22	50.293	16.728	52.726	8.119
DQ11	0.89	49.694	16.935	0.148	7.867

FIG. 3A

4/22

Compound	Dielectric Energy (kcal)/mole) G	Steric Energy (kcal/mole) H	Total Energy (Hartree) I	Heat of Formation (kcal/mole)	HOMO Energy (ev)
DQ 18	7.7	39.331	214.593	258.295	13.703
DQ 16	7.211	39.597	221.775	242.427	13.635
DQ 10	6.602	40.322	236.121	218.102	13.52
DQ 14	8.438	39.924	205.938	291.32	13.855
DQ 17	7.759	50.797	329.153	171.131	12.628
DQ 15	7.301	49.902	336.331	155.69	12.601
DQ 12	6.62	50.899	350.679	131.143	12.552
DQ 13	8.487	50.293	320.496	204.337	12.687
DQ11	8.312	49.694	321.968	190.296	12.661

FIG. 3B

5/22

Compound	Ionization Potential (eV) L	Log P M	LUMO (eV) Energy N	Shape Index (basic kappa, order 3) O	Valence Connectivity Index (order 2, standard) Q	Solvent Accessible Surface Area (Å <sup>2</sup> ) P
DQ 18	13.703	6.409	-7.127	21.031	521.24	11.069
DQ 16	13.635	6.86	-6.601	22.027	539.815	11.423
DQ 10	13.52	7.653	-5.948	23.967	576.054	12.13
DQ 14	13.855	6.179	-8.122	13.04	485.397	10.53
DQ 17	12.628	12.75	-7.139	36.681	813.7	16.726
DQ 15	12.601	13.201	-6.598	37.686	831.853	17.08
DQ 12	12.552	13.993	5.946	39.658	883.721	17.787
DQ 13	12.687	12.52	-8.119	26.747	778.615	16.187
DQ11	12.661	12.697	-7.867	35.716	793.278	16.372

FIG. 3C

6/22

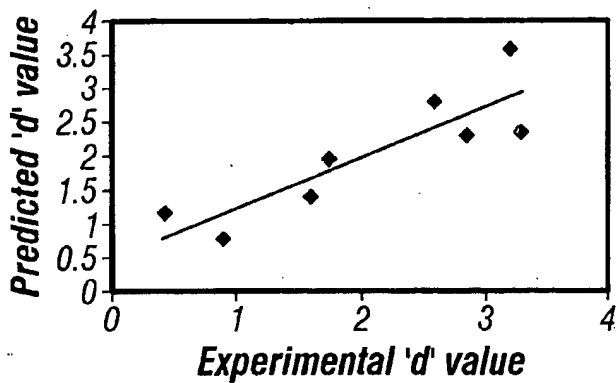


FIG. 4A

Predictive Eq. for Pd II

$$B = 0.0554277 * E + 0.610452 * L - 16.7616 / N - 9.0729$$

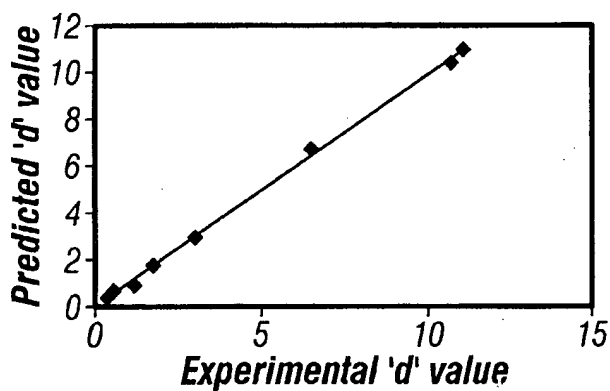


FIG. 4B

Predictive Eq. for Pd IV

$$B = 71.6336 * D + 0.463796 * E + 23.6272 * F + 19.8848 * G - 9.37422 * H + 2.71931 * I + 108.256$$

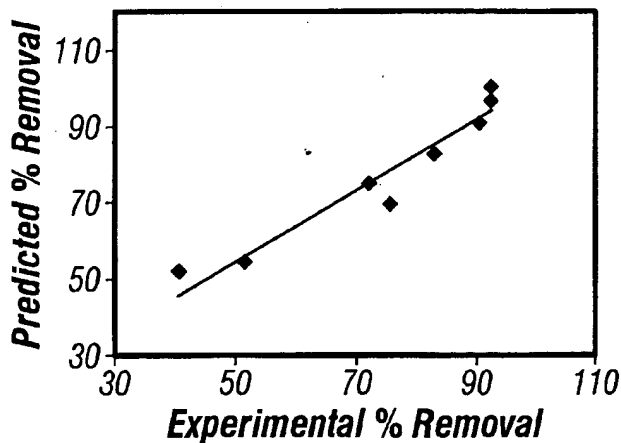
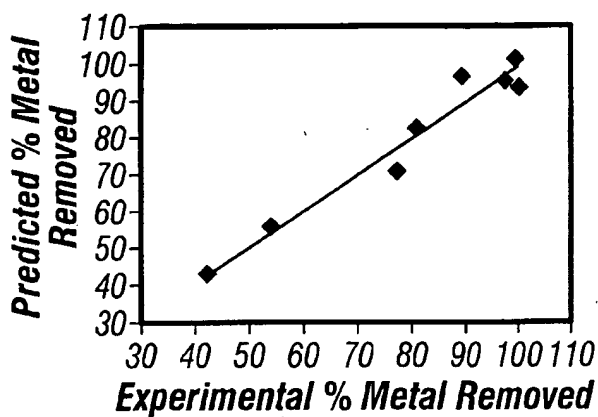


FIG. 4C

Predictive Eq. for Pt II

$$B = -276.194 * L - 69.6714 * M - 4.68162 * N - 7.67628 * O + 3.7778 * P - 154.864 * Q + 4211.14$$

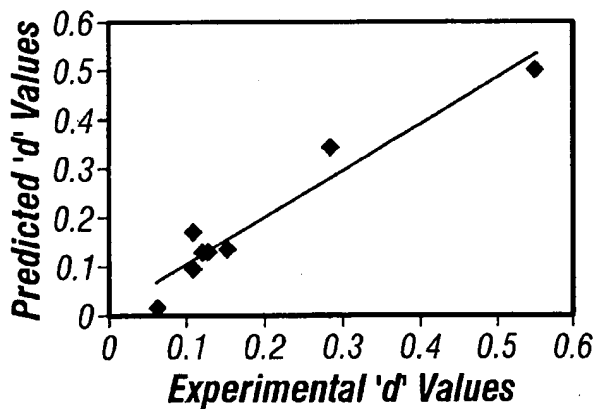
7/22



*Predictive Eq. for Pt IV*

$$\begin{aligned}
 B = & 283.378 * D + 1.4239 \\
 & 9 * E + 173.825 * F + 212.2 \\
 & 66 * G + 2.69479 * H + 14 \\
 & 4354 * I + 167.3
 \end{aligned}$$

FIG. 4D



*Predictive Eq. for Rh III*

$$\begin{aligned}
 B = & 0.00584793 * E - \\
 & 0.90334 * N - 42.1486 / N - \\
 & 12.3346
 \end{aligned}$$

FIG. 4E

8/22

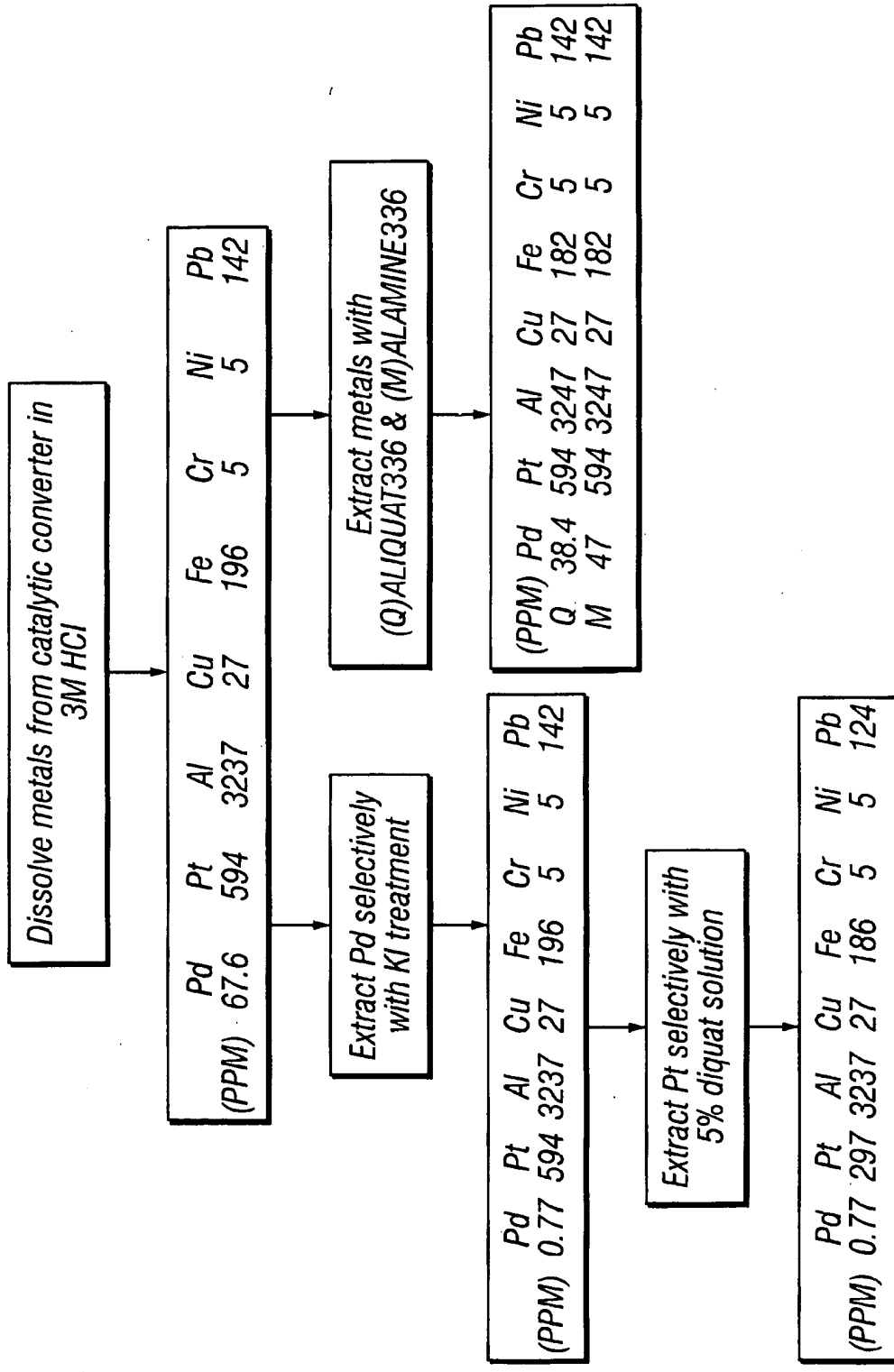


FIG. 5



9/22

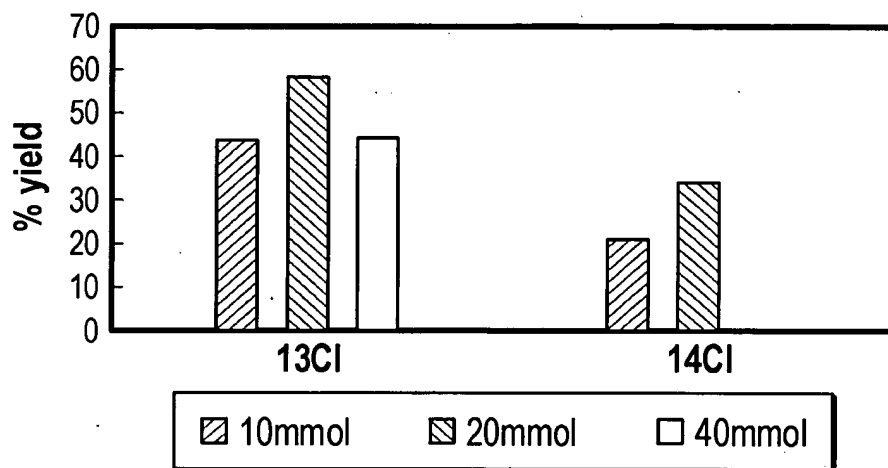


FIG. 6

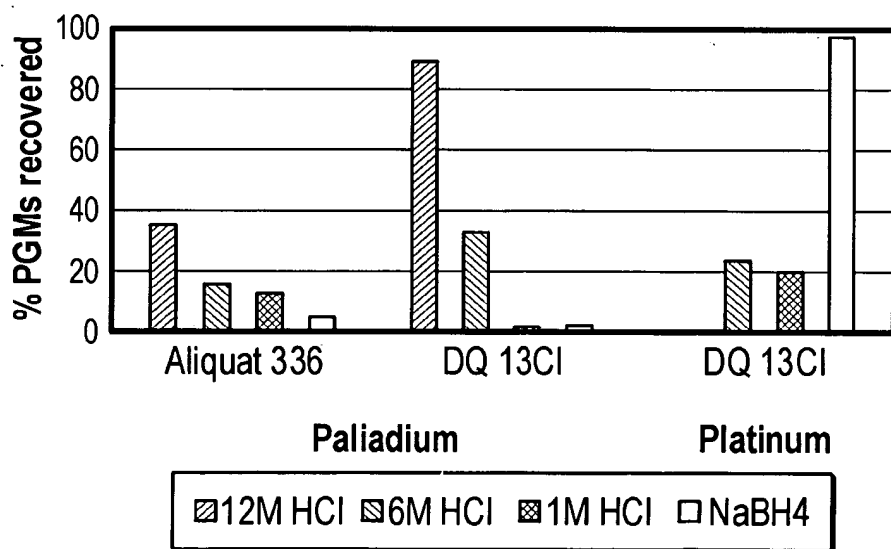
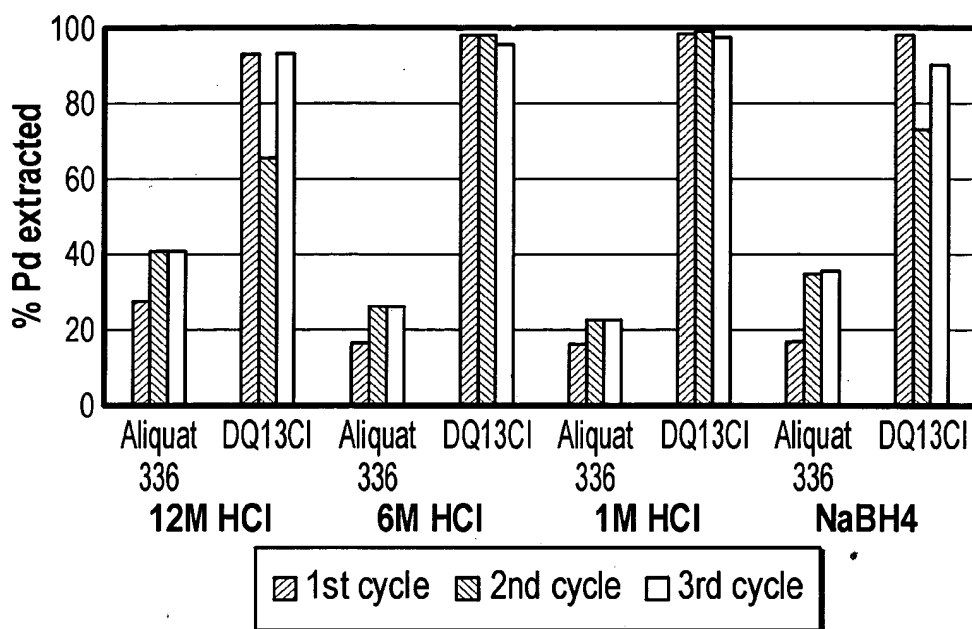
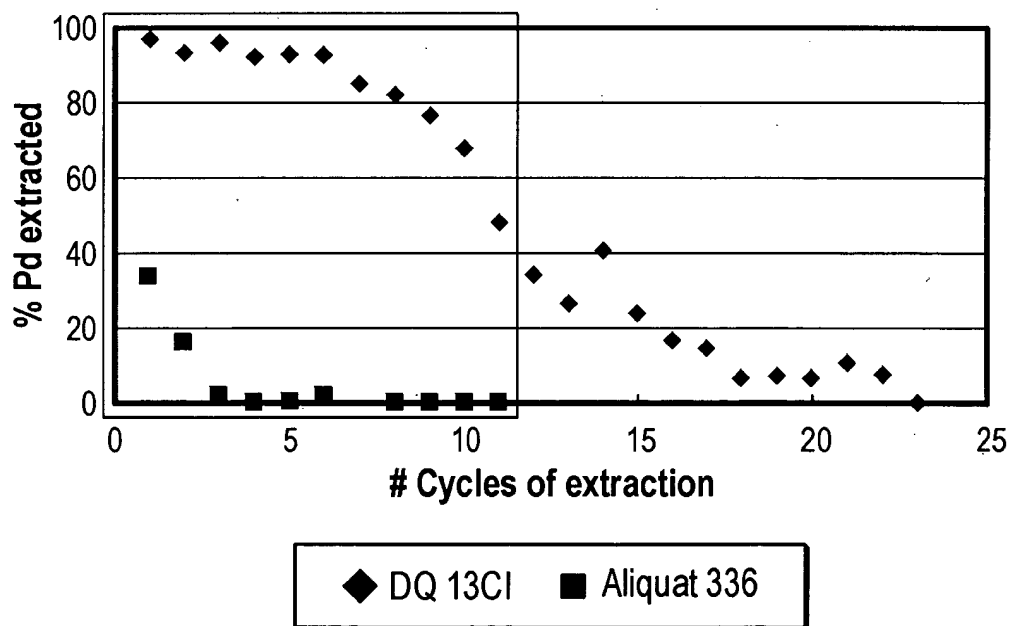


FIG. 7

**10/22**

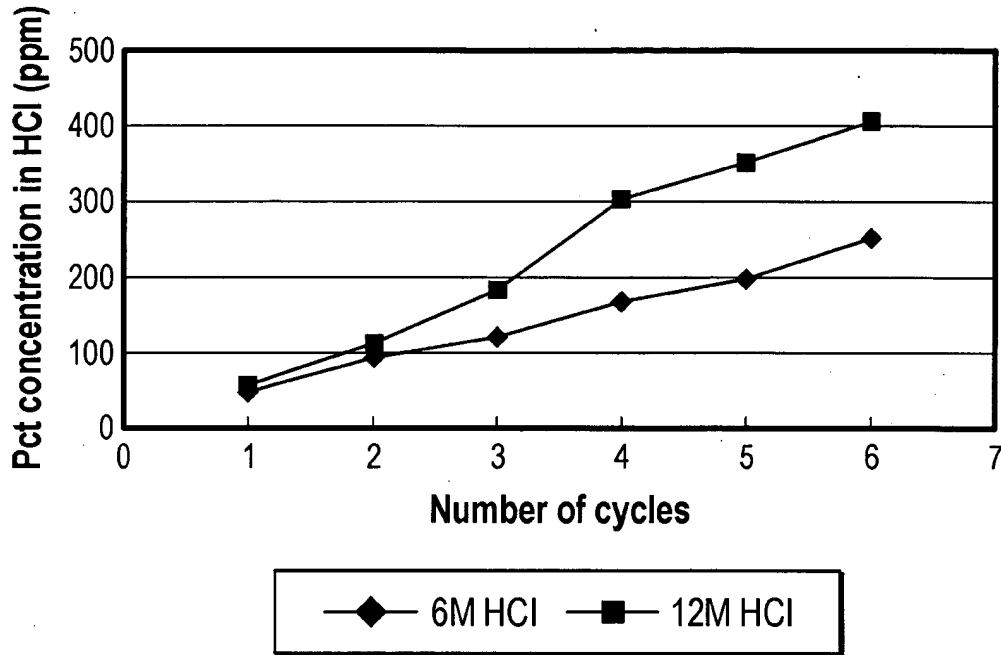


**FIG. 8**

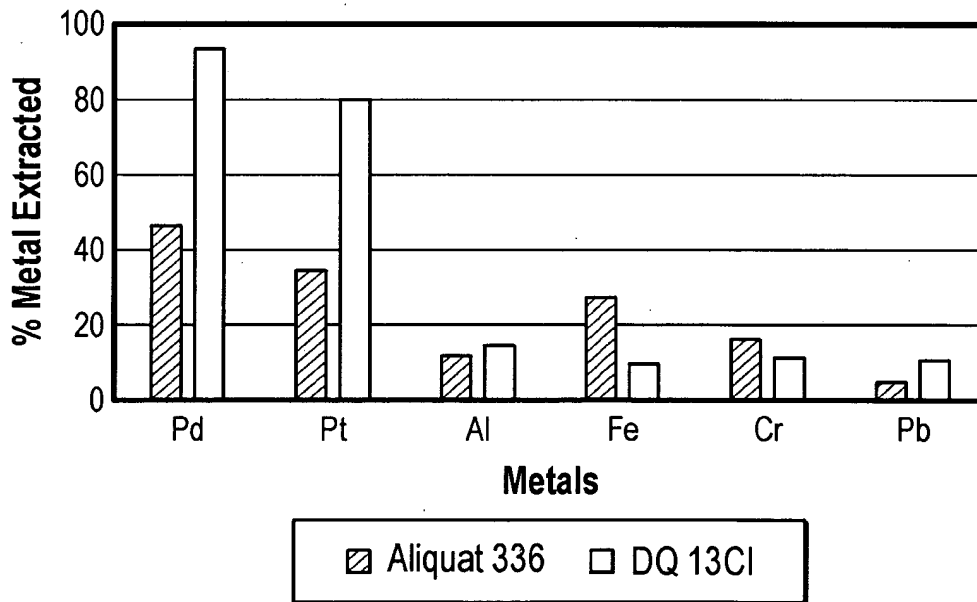


**FIG. 9**

**11/22**

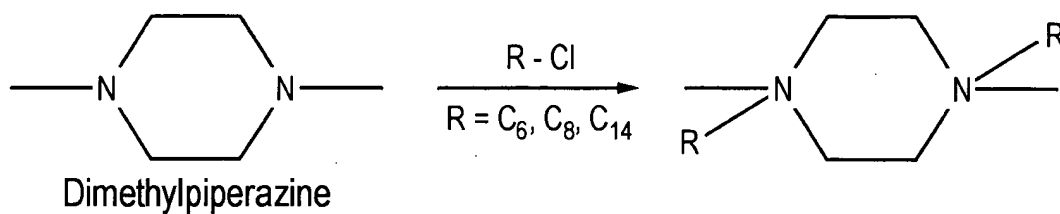


**FIG. 10**

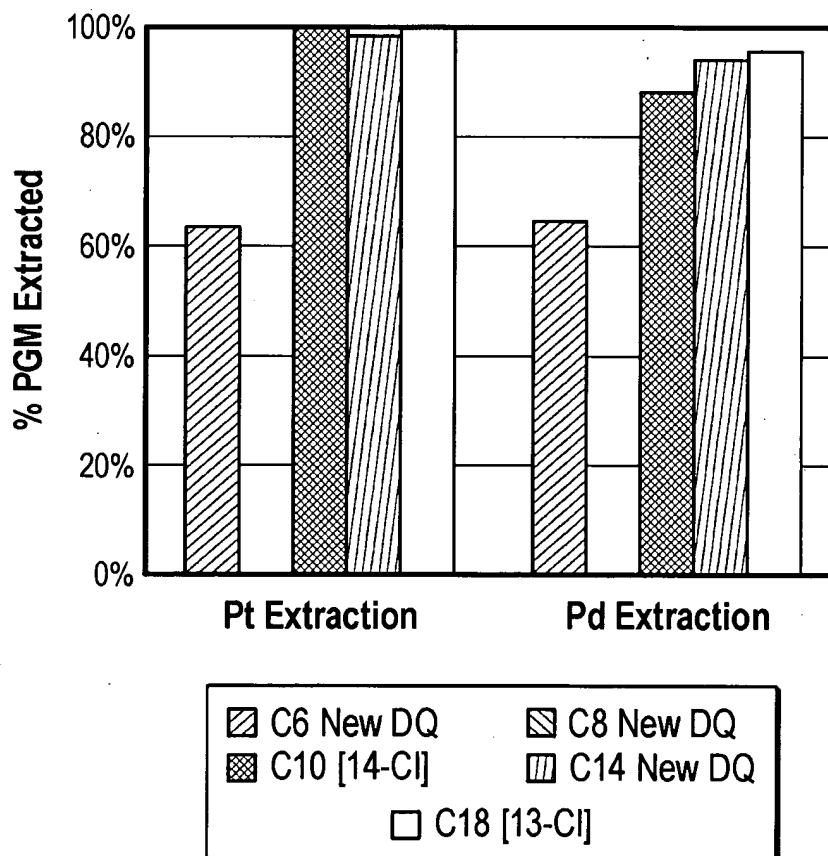


**FIG. 11**

**12/22**

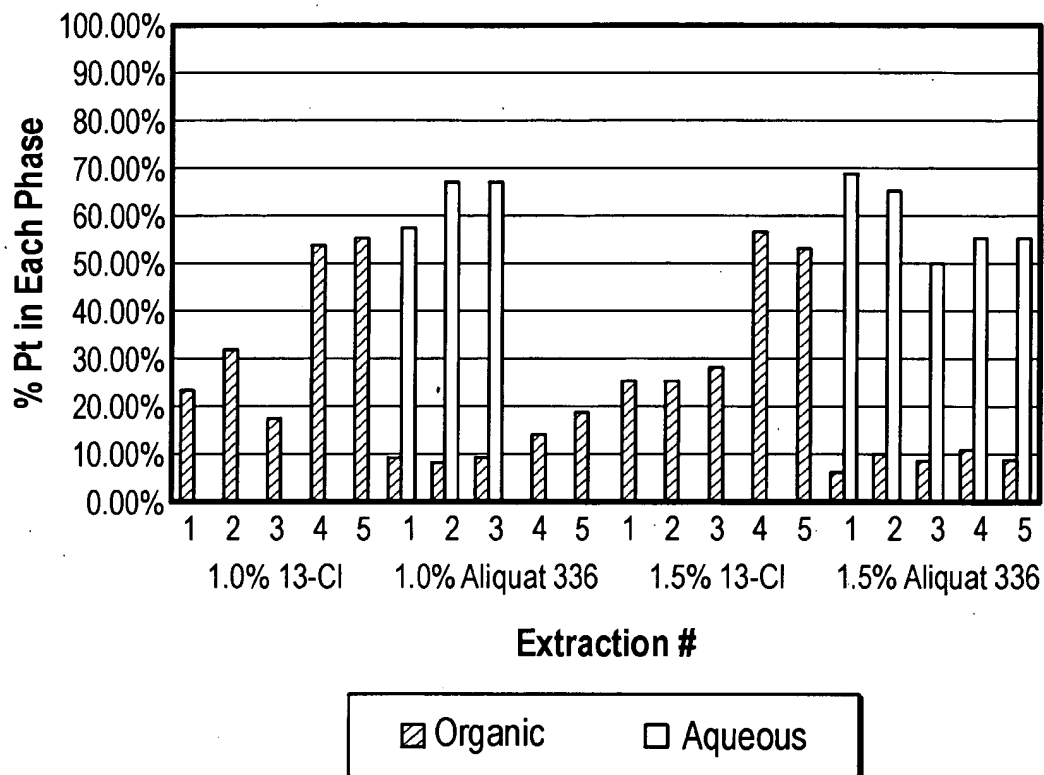


**FIG. 12**

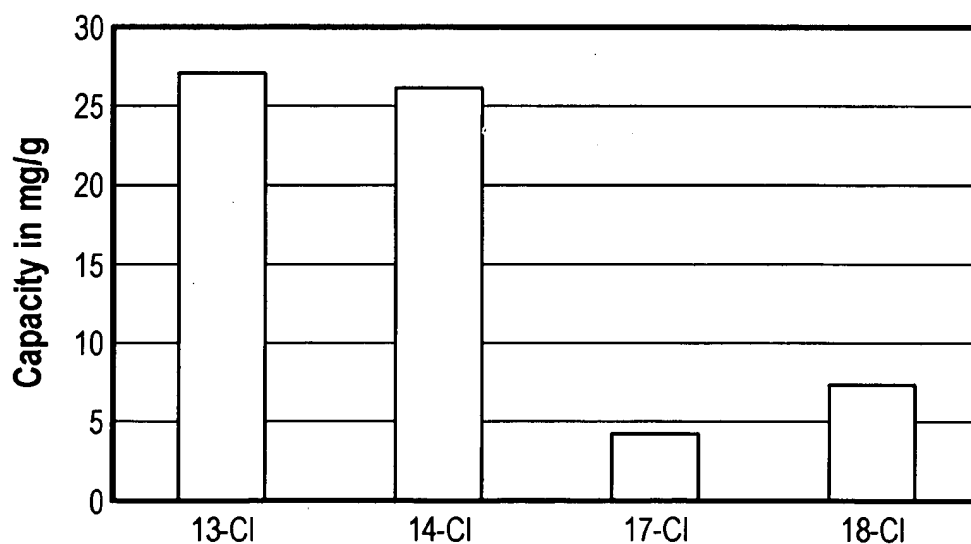


**FIG. 13**

**13/22**



**FIG. 14**



**FIG. 15**

14/22

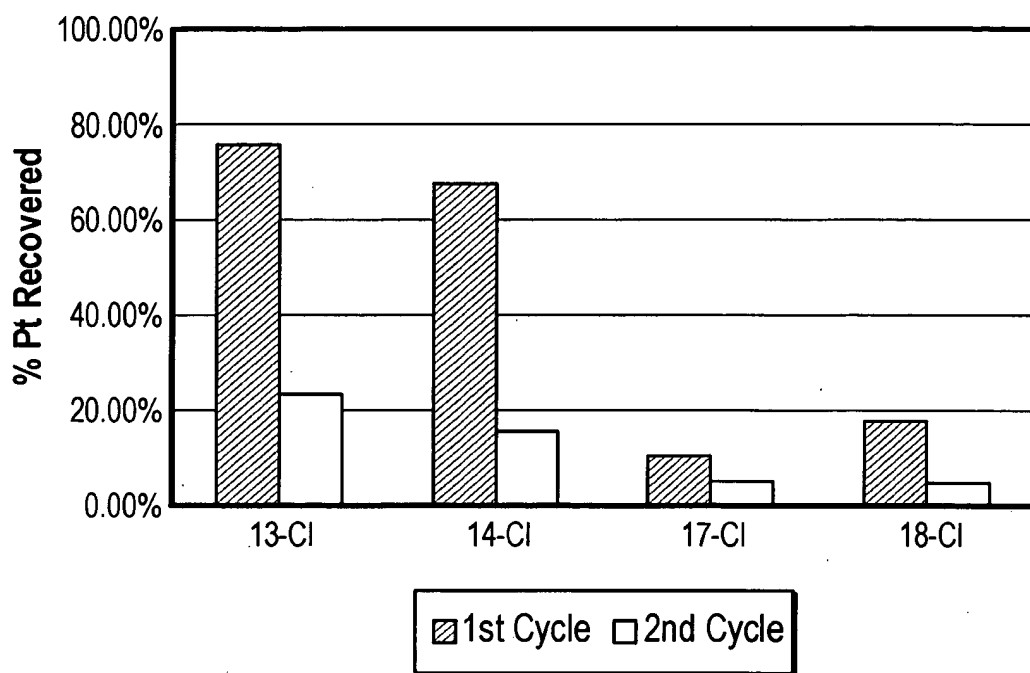


FIG. 16

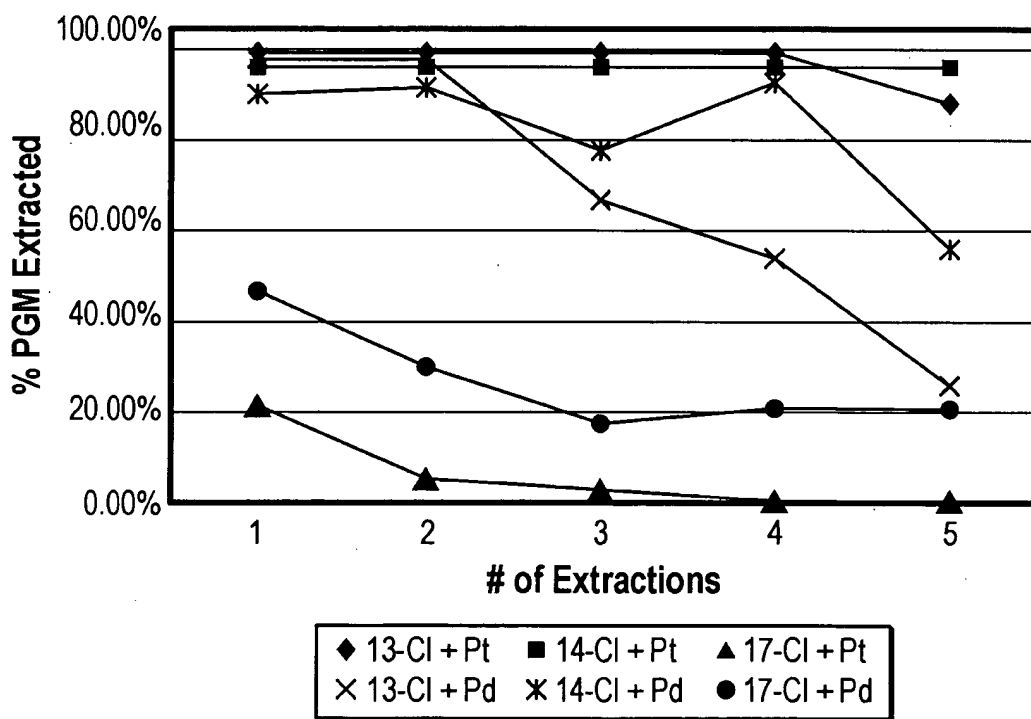
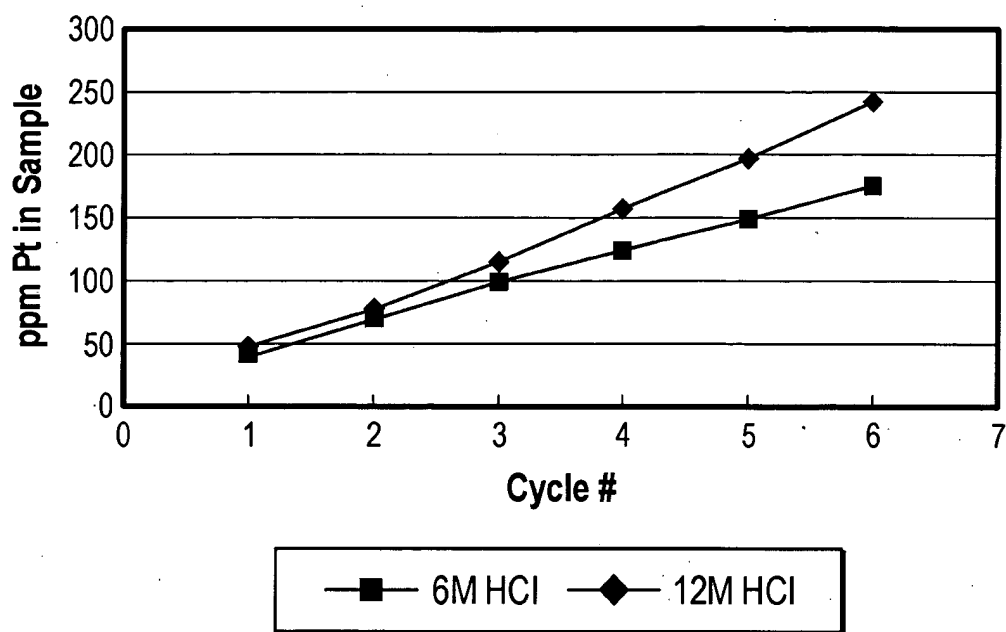
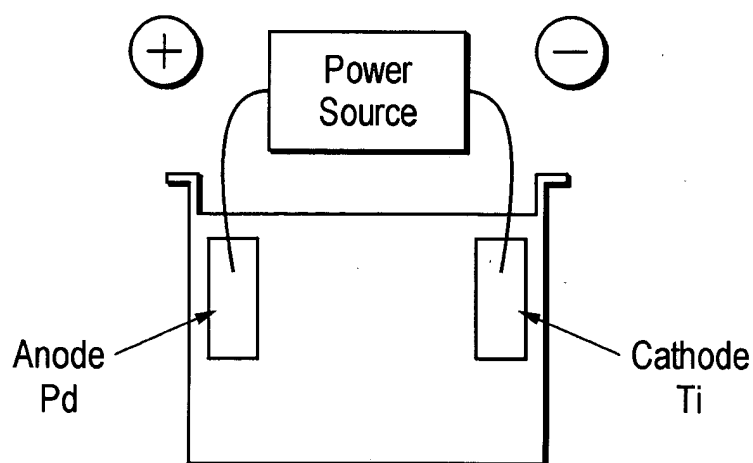


FIG. 17

**15/22**



**FIG. 18**



**FIG. 19**

16/22

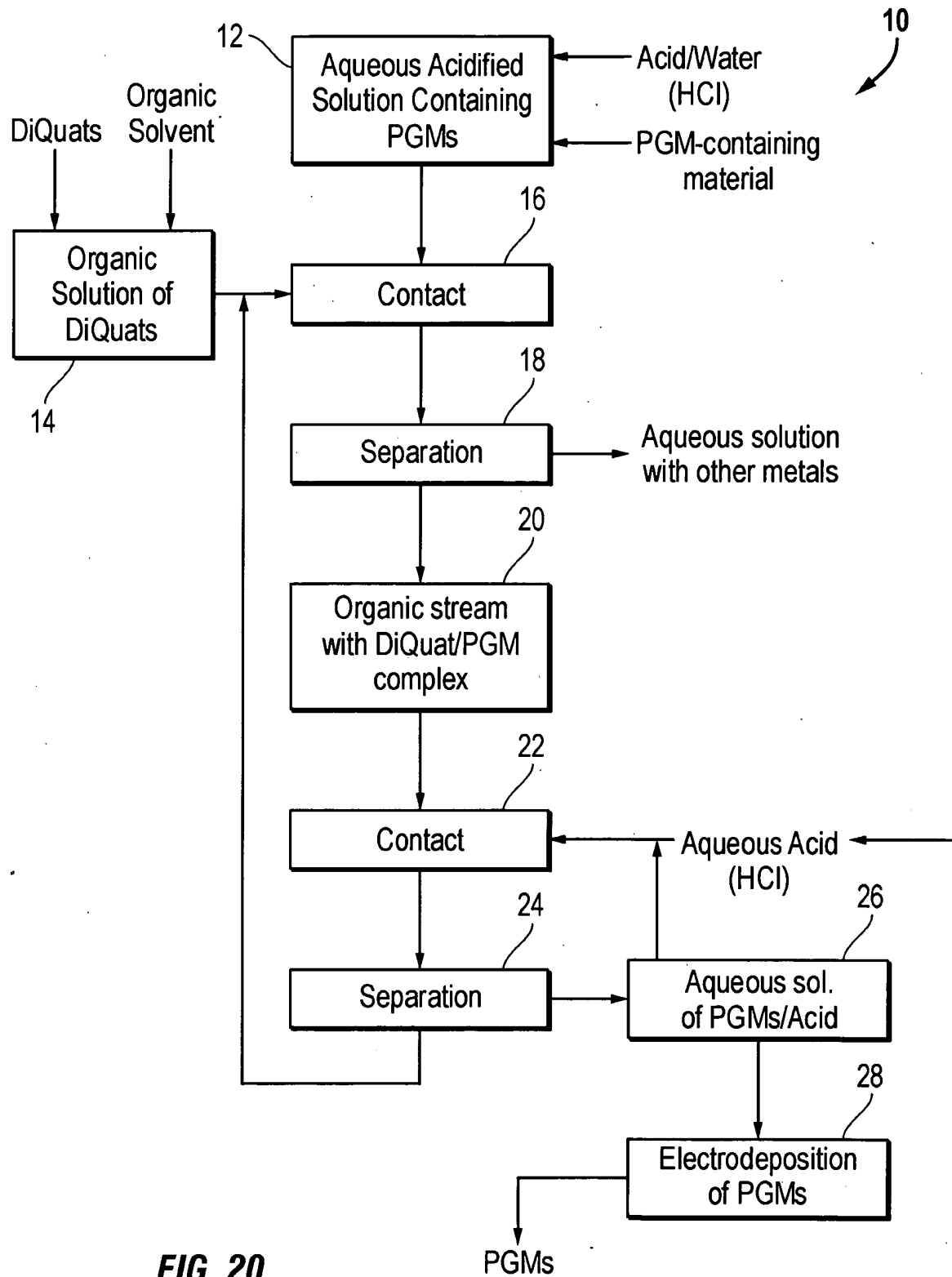
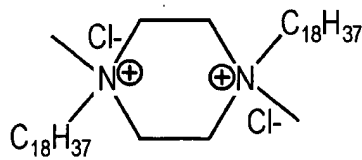


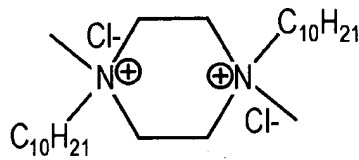
FIG. 20



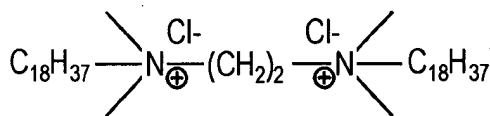
17/22



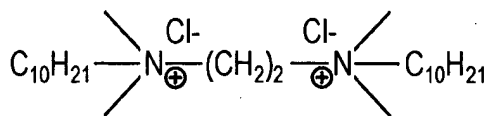
DQ 13-Cl



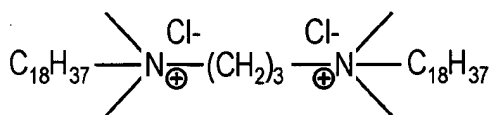
DQ 14-Cl



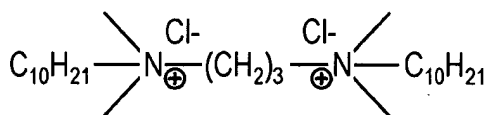
DQ 11-Cl



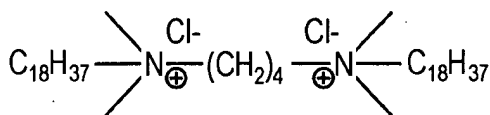
DQ 9-Cl



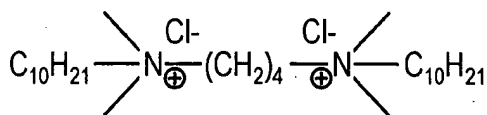
DQ 17-Cl



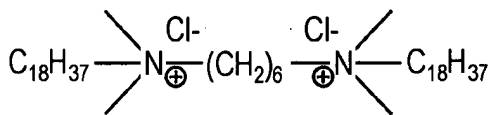
DQ 18-Cl



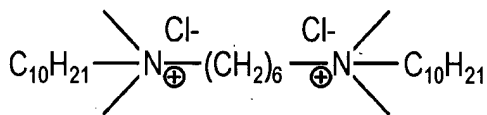
DQ 15-Cl



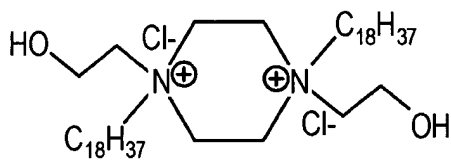
DQ 16-Cl



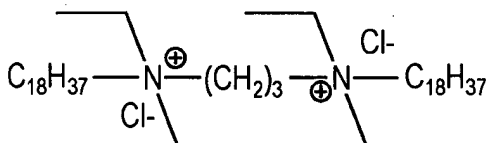
DQ 12-Cl



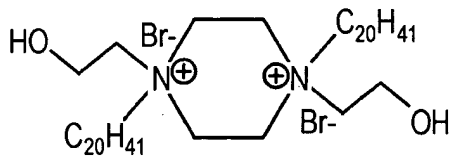
DQ 10-Cl



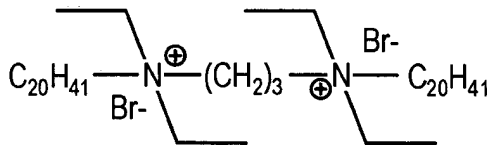
DQ C18-HyPip



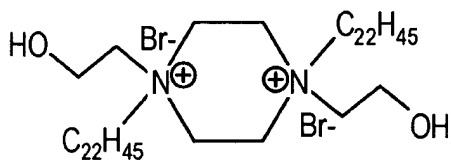
DQ C18-Et4Me3



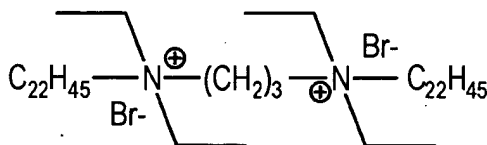
DQ C20Br-HyPip



DQ C20Br-Et4Me3



DQ C22Br-HyPip



DQ C22Br-Et4Me3

FIG. 21

18/22

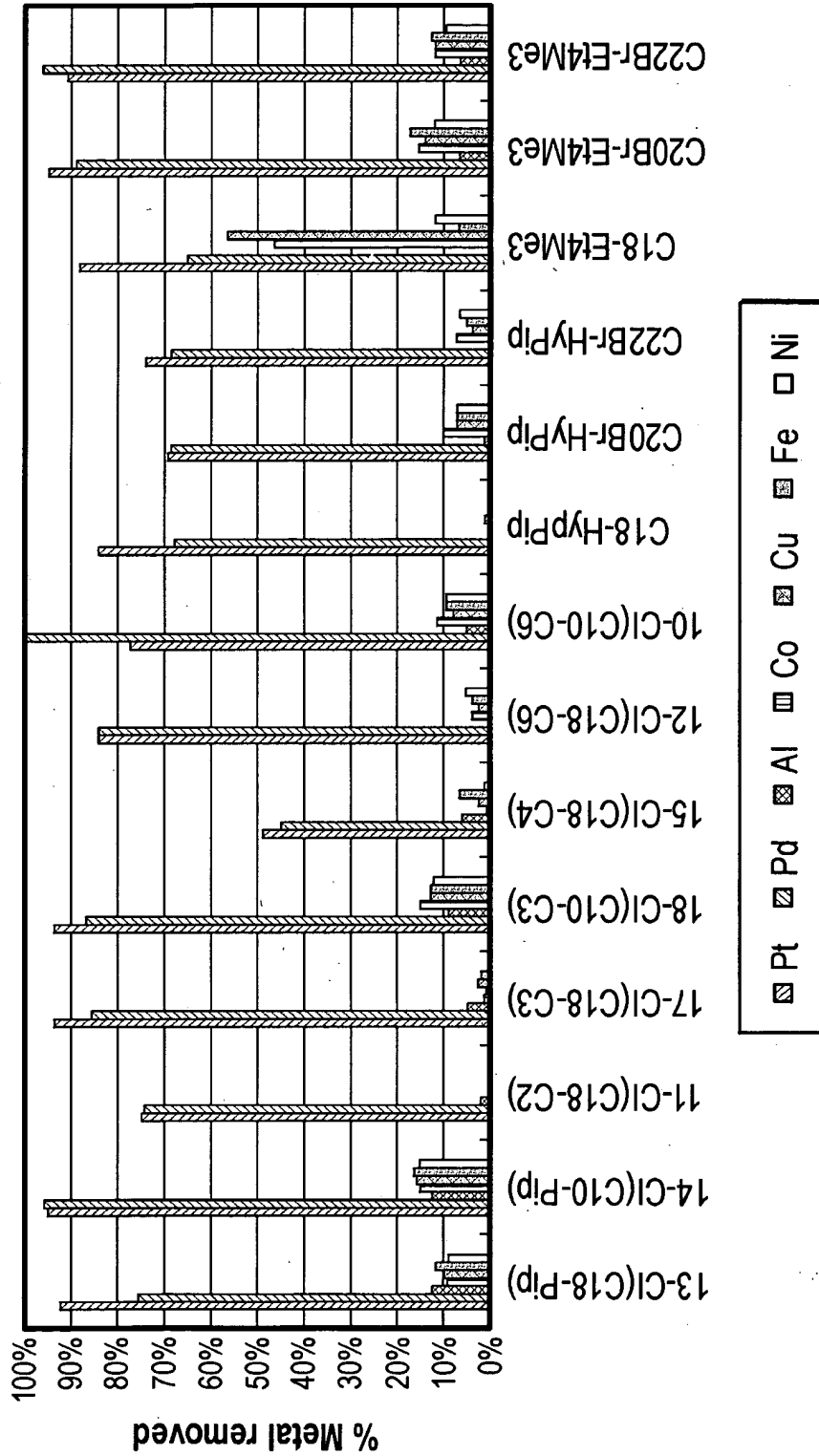
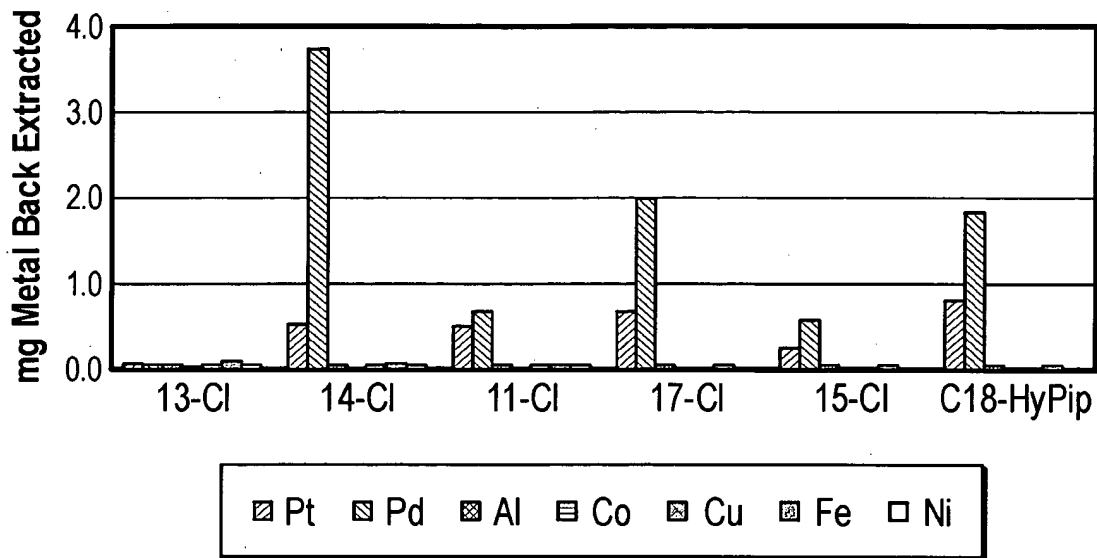
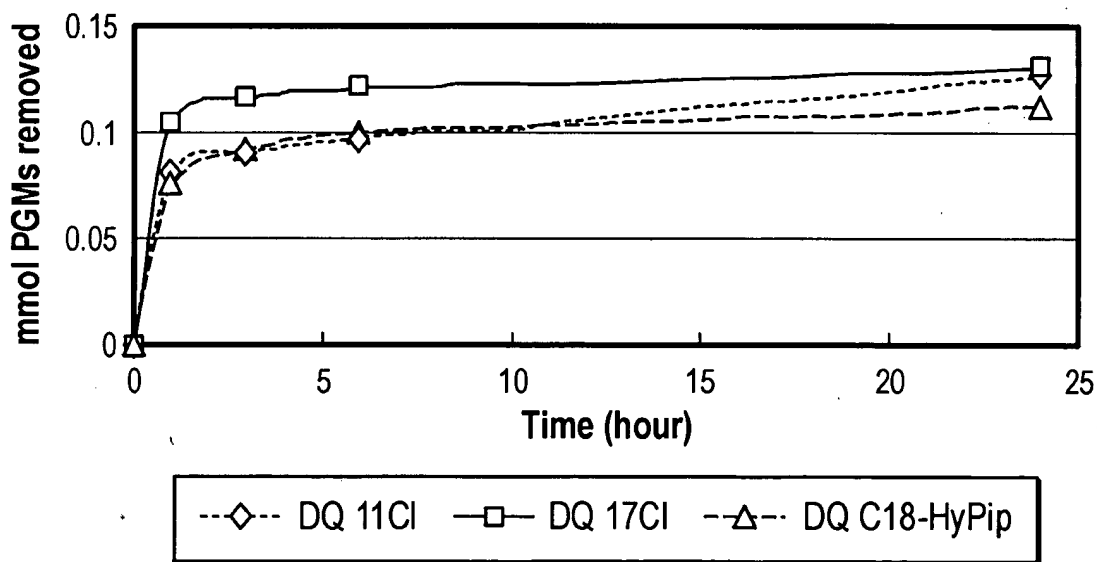


FIG. 22

**19/22**

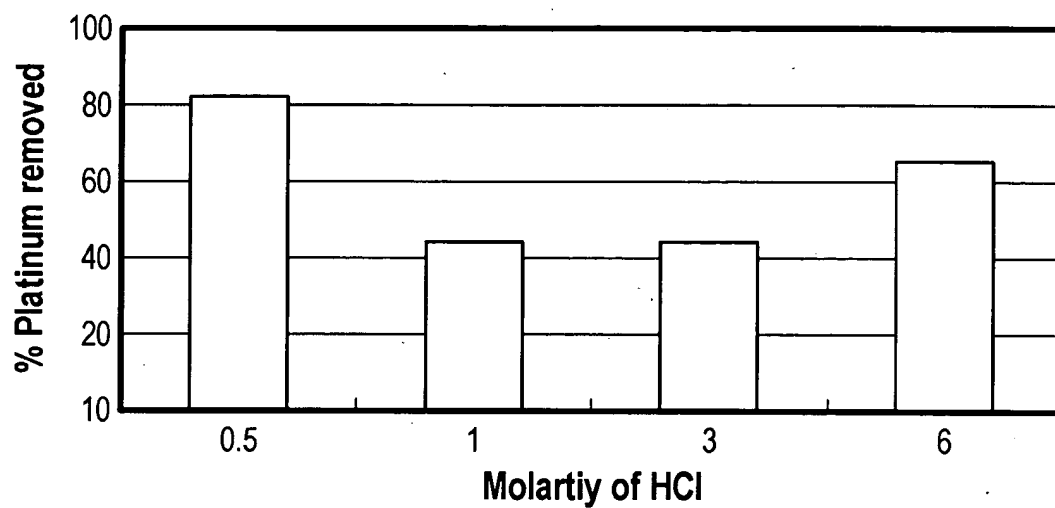


**FIG. 23**

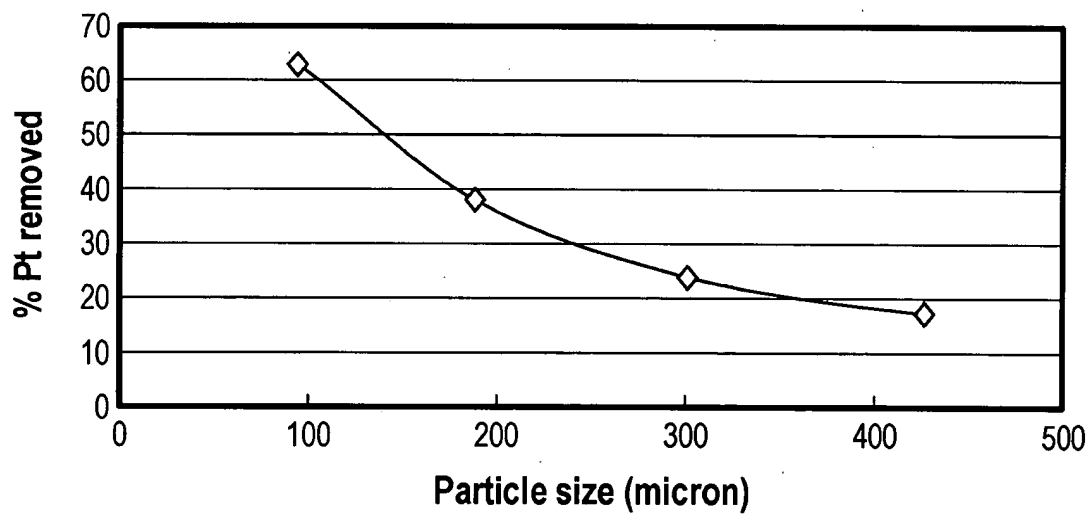


**FIG. 24**

**20/22**



**FIG. 25**



**FIG. 26**

21/22

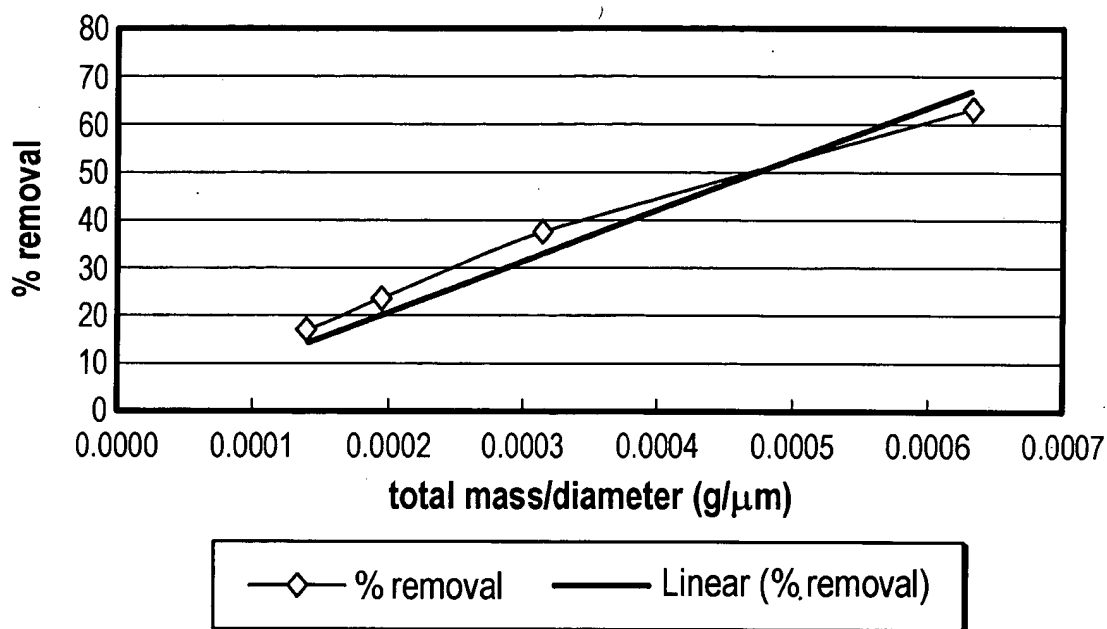


FIG. 27

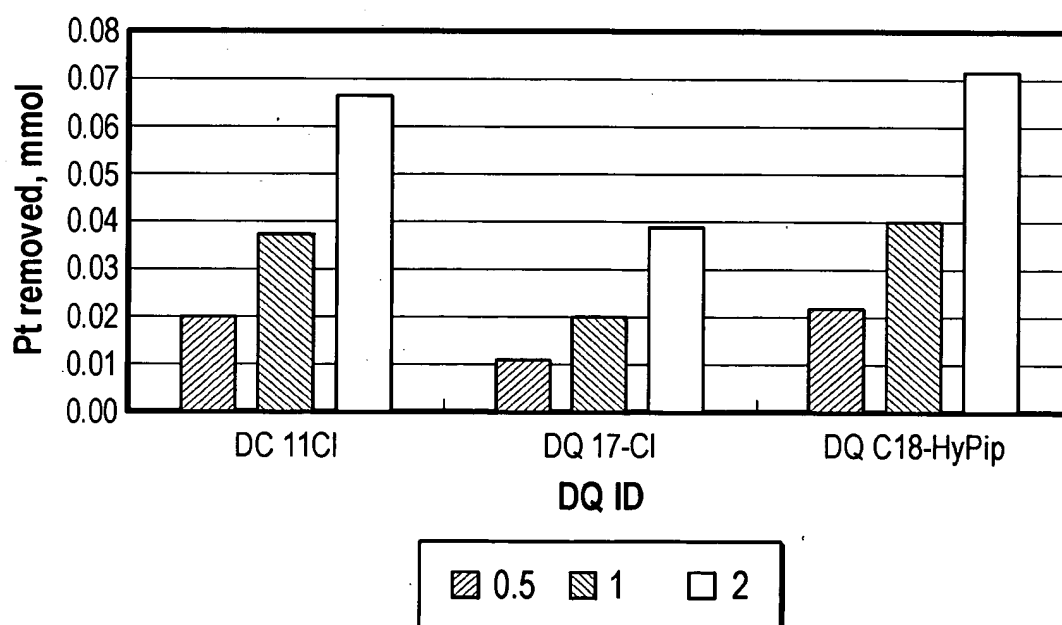
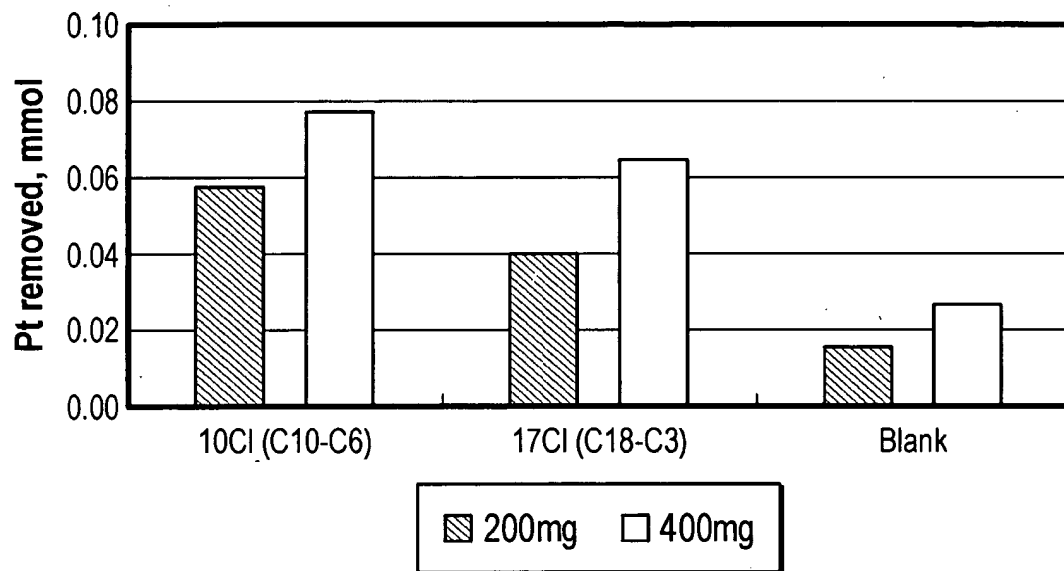


FIG. 28

**22/22**



**FIG. 29**